Electronic Supporting Information for *'Molecular dynamics simulations of structure and dynamics of organic molecular crystals'*

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S.1 Definition of some variables calculated in the simulations

Average atomic positions. For atom i, with positional vector $\mathbf{R_{i,fr}} = (x_{i,fr}, y_{i,fr}, z_{i,fr})$ at a particular frame *fr* of a trajectory with *N* frames average atomic positions are:

$$\langle \mathbf{R_i} \rangle = (\langle x_i \rangle, \langle y_i \rangle, \langle z_i \rangle), \tag{1}$$

where angle brackets denote averaging over the length of simulation, $\langle x_i \rangle$ is defined as

$$\langle x_i \rangle = \frac{\sum_{fr=1}^{N} x_{i,fr}}{N}, \tag{2}$$

and $\langle y_i \rangle$ and $\langle z_i \rangle$ are obtained analogously.

Bond lengths from average positions. Bond length from average positions for atoms i and j is:

$$d(\langle \mathbf{R_i} \rangle, \langle \mathbf{R_j} \rangle) = \| \langle \mathbf{R_j} \rangle - \langle \mathbf{R_i} \rangle \| \tag{3}$$

Average bond legths Average bond lengths for atom i and j are:

$$\langle d(\mathbf{R_i}, \mathbf{R_j}) \rangle = \frac{\sum_{\mathbf{fr}=1}^{\mathbf{N}} \| \mathbf{R_{j,fr}} - \mathbf{R_{i,fr}} \|}{\mathbf{N}} \tag{4}$$

Mean sqaure displacements of atoms

$$msd_x = U_{11}^C = \frac{\sum_{fr=1}^{N} (x_{i,fr} - \langle x_i \rangle)^2}{N}, \tag{5}$$

where msd_x is the mean square displacemnet of an atom in the x directions, and mean square displacements in y and z directions are calculated analogously for y and z.

S.2 Arrhenius activation energies for benzene

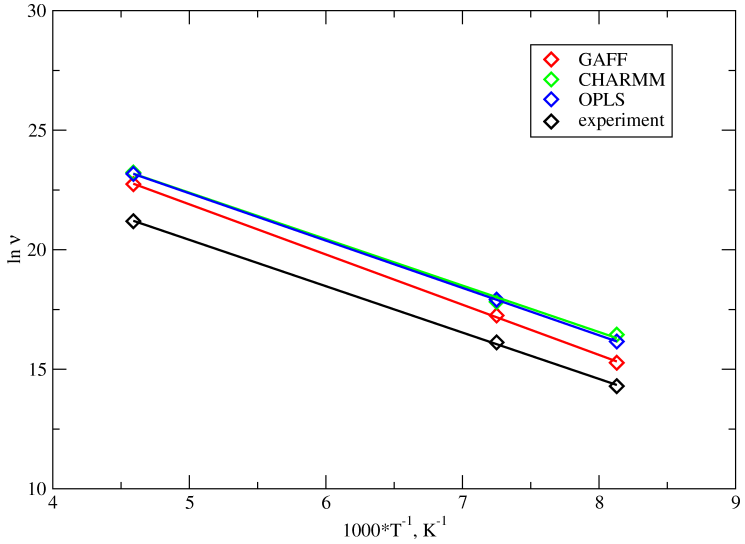

Figure S1: Natural logarithm of reorientation frequency versus inverse temperature for benzene as simulated by GAFF, CHARMM, OPLS compared to experimental data.

From plot shown on Figure S1 and using the Arrhenius equation in the transition state theory form:

$$k = \frac{k_B T}{h} e^{\frac{-\Delta G^{\ddagger}}{RT}} = \frac{k_B T}{h} e^{\frac{\Delta S^{\ddagger}}{R} - \frac{\Delta H^{\ddagger}}{RT}} \tag{6}$$

one can obtain:

$$\Delta H^{\ddagger} = -R \frac{\Delta lnk}{\Delta T^{-1}} \tag{7}$$

$$\Delta S^{\ddagger} = R(lnk(0) - ln\frac{k_B T}{h}) \tag{8}$$

$$\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger} \tag{9}$$

where $\Delta H^{\ddagger}, \Delta S^{\ddagger}, \Delta G^{\ddagger}$ are the enthalpy, entropy and free energy of activation, respectively, R is the gas constant, $\frac{\Delta lnk}{\Delta T^{-1}}$ is the slope of the line, $lnk(0)$ is the intercept of the line with the y-axis, k_B is Boltzmann constant and h is Planck's constant.

S.3 Simulation data

Tables S1-S11 contain data on the size of the supercell, bond lengths from average positions, average bond lengths and equivalent ADPs for the model compounds used in the study.

Tables S12-S15 and Figure S2 contain bond lengths from average positions and ADPs for heavy atoms of AGA from the preliminary study on the effect of length, size and cutoff for non-bonded interactions on the effect of simulations.

In all tables atom names from the corresponding cif files were used. All bond lengths are given in Å , and U_{eq} - in $Å^2$.

Table S1. Benzene 123 K

supercell 4 x 3 x 4, 29.592 x 28.305 x 27.112 A, 192 molecules, 2304 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3[1]	experiment
a, Å	7.406(8)	7.451(8)	7.413(8)	7.537(5)	7.398(2)
b, Å	9.445(11)	9.503(11)	9.455(10)	9.612(7)	9.435(2)
c, Å	6.785(8)	6.827(8)	6.792(7)	6.906(5)	6.778(1)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
C1-C2	1.3935(157)	1.4012(177)	1.4081(159)	1.3425(161)
C2-C3	1.3939(158)	1.4016(177)	1.4085(159)	1.3426(161)
C1-C3'	1.3934(157)	1.4012(177)	1.4079(159)	1.3423(161)
C1-D1	1.0881(194)	1.0805(185)	1.0807(186)	1.1047(185)
C2-D2	1.0884(194)	1.0810(185)	1.0811(186)	1.1051(186)
C3-D3	1.0871(194)	1.0800(185)	1.0801(186)	1.1045(186)

1 only first 6000 frames used

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
C1-C2	1.3872(4)	1.3939(4)	1.4010(4)	-	1.3943(11)
C2-C3	1.3868(4)	1.3937(4)	1.4005(4)	-	1.3954(11)
C1-C3'	1.3861(4)	1.3926(4)	1.3998(4)	-	1.3922(11)
C1-D1	1.0818(4)	1.0734(5)	1.0737(5)	-	1.0837(13)
C2-D2	1.0807(4)	1.0720(4)	1.0725(4)	-	1.0851(13)
C3-D3	1.0803(5)	1.0721(4)	1.0725(4)	-	1.0825(13)

Ueq

	gaff	charmm	opls	mm3	experiment
C1	0.0219(3)	0.0226(3)	0.0220(3)	-	0.0231(3)
C2	0.0229(3)	0.0238(3)	0.0232(3)	-	0.0238(3)
C3	0.0221(3)	0.0229(3)	0.0223(3)	-	0.0233(3)
D1	0.0346(4)	0.0370(4)	0.0362(4)	-	0.0418(5)
D2	0.0374(5)	0.0407(4)	0.0395(4)	-	0.0439(5)
D3	0.0352(5)	0.0381(5)	0.0369(4)	-	0.0426(5)

Table S2. Benzene 138 K

supercell 4 x 3 x 4, 29.56 x 28.26 x 27.24 A, 192 molecules, 2304 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	7.406(9)	7.450(9)	7.413(9)	7.569(15)	7.39
b, Å	9.440(12)	9.497(12)	9.450(11)	9.648(19)	9.42
c, Å	6.832(8)	6.873(8)	6.839(8)	6.975(14)	6.81
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
C1-C2	1.3936(167)	1.4014(188)	1.4082(168)	1.3426(167)
C2-C3	1.3939(167)	1.4018(188)	1.4085(168)	1.3426(167)
C1-C3'	1.3934(167)	1.4012(188)	1.4079(168)	1.3425(167)
C1-H1	1.0881(205)	1.0806(200)	1.0808(200)	1.105(20)
C2-H2	1.0884(205)	1.0810(200)	1.0811(200)	1.105(20)
C3-H3	1.0872(205)	1.0801(201)	1.0802(200)	1.105(20)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
C1-C2	1.3861(4)	1.3926(4)	1.3997(4)	-	1.392(7)
C2-C3	1.3856(4)	1.3924(5)	1.3992(4)	-	1.397(7)
C1-C3'	1.3848(4)	1.3913(4)	1.3984(4)	-	1.391(7)
C1-H1	1.0807(5)	1.0723(4)	1.0724(4)	-	1.095(8)
C2-H2	1.0796(4)	1.0707(4)	1.0712(4)	-	1.087(10)
C3-H3	1.0794(4)	1.0710(4)	1.0712(4)	-	1.076(9)

Ueq

atom	gaff	charmm	opls	mm3	experiment
C1	0.0258(3)	0.0266(4)	0.0261(3)	-	0.024
C2	0.0269(4)	0.0279(4)	0.0273(4)	-	0.025
C3	0.0260(4)	0.0269(4)	0.0263(4)	-	0.026
H1	0.0408(5)	0.0436(5)	0.0429(5)	-	0.043
H2	0.0439(5)	0.0475(6)	0.0464(5)	-	0.055
H3	0.0414(5)	0.0445(5)	0.0434(5)	-	0.048

Table S3. Benzene 218 K

supercell 4 x 3 x 4, 29.76 x 28.65 x 27.68 A, 192 molecules, 2304 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	7.471(14)	7.513(14)	7.474(14)	7.746(78)	7.44
b, Å	9.589(18)	9.644(18)	9.594(18)	9.942(100)	9.55
c, Å	6.949(13)	6.988(13)	6.952(13)	7.204(73)	6.92
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
C1-C2	1.3939(210)	1.4019(236)	1.4085(212)	1.3431(207)
C2-C3	1.3939(210)	1.4019(236)	1.4085(212)	1.3431(207)
C1-C3'	1.3939(210)	1.4019(236)	1.4085(212)	1.3432(207)
C1-H1	1.0882(257)	1.0809(252)	1.0810(251)	1.1065(252)
C2-H2	1.0883(257)	1.0809(252)	1.0810(251)	1.1065(252)
C3-H3	1.0883(257)	1.0809(252)	1.0810(251)	1.1065(252)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
C1-C2	1.3763(5)	1.3803(6)	1.3882(6)	-	1.394(10)
C2-C3	1.3758(5)	1.3800(6)	1.3876(5)	-	1.387(9)
C1-C3'	1.3742(6)	1.3784(6)	1.3861(5)	-	1.389(9)
C1-H1	1.0723(5)	1.0616(5)	1.0625(5)	-	1.059(15)
C2-H2	1.0704(5)	1.0595(6)	1.0605(5)	-	1.085(17)
C3-H3	1.0708(5)	1.0603(5)	1.0612(5)	-	1.072(16)

Ueq

atom	gaff	charmm	opls	mm3	experiment
C1	0.0573(9)	0.0594(8)	0.0573(8)	-	0.045
C2	0.0593(9)	0.0614(8)	0.0593(8)	-	0.048
C3	0.0577(9)	0.0598(8)	0.0576(8)	-	0.046
H1	0.0918(12)	0.1012(15)	0.0971(13)	-	0.082
H2	0.0977(12)	0.1072(12)	0.1029(13)	-	0.086
H3	0.0931(13)	0.1025(17)	0.0980(13)	-	0.079

Table S4. Isopropylcyclohexane 150 K

supercell 2 x 6 x 3, 31.378 x 31.788 x 31.923 A, 144 molecules, 3888 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	15.617(15)	15.615(17)	15.504(16)	16.082(13)	15.689(8)
b, Å	5.274(5)	5.273(6)	5.235(6)	5.431(4)	5.298(3)
c, Å	10.592(10)	10.591(12)	10.515(11)	10.908(9)	10.641(6)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	101.79	101.79	101.79	101.79	101.79
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
C1-C2	1.551(22)	1.547(23)	1.545(23)	1.545(23)
C1-C6	1.553(22)	1.548(23)	1.546(23)	1.545(23)
C1-C7	1.562(21)	1.528(23)	1.552(23)	1.556(24)
C1-H11	1.094(22)	1.116(22)	1.092(21)	1.120(22)
C2-C3	1.543(22)	1.535(22)	1.537(23)	1.538(23)
C2-H21	1.093(22)	1.112(22)	1.091(22)	1.116(22)
C2-H22	1.092(22)	1.111(22)	1.090(22)	1.115(22)
C3-C4	1.541(22)	1.532(22)	1.534(23)	1.536(22)
C3-H31	1.091(22)	1.112(22)	1.090(22)	1.116(22)
C3-H32	1.092(22)	1.113(22)	1.090(22)	1.116(22)

C4-C5	1.543(22)	1.534(22)	1.536(23)	1.537(22)
C4-H41	1.091(22)	1.112(22)	1.090(22)	1.116(22)
C4-H42	1.093(22)	1.114(22)	1.091(22)	1.116(22)
C5-C6	1.543(22)	1.537(22)	1.537(23)	1.539(23)
C5-H51	1.093(22)	1.113(22)	1.091(22)	1.116(22)
C5-H52	1.092(22)	1.112(22)	1.090(22)	1.116(22)
C6-H61	1.092(22)	1.112(22)	1.090(22)	1.115(22)
C6-H62	1.092(22)	1.111(22)	1.090(22)	1.115(22)
C7-C8	1.548(22)	1.541(23)	1.539(23)	1.543(23)
C7-C9	1.545(22)	1.540(23)	1.536(23)	1.543(23)
C7-H71	1.093(21)	1.117(22)	1.092(22)	1.120(22)
C8-H81	1.092(22)	1.111(22)	1.090(22)	1.115(22)
C8-H82	1.091(22)	1.109(22)	1.089(22)	1.113(22)
C8-H83	1.092(22)	1.110(22)	1.089(22)	1.114(21)
C9-H91	1.092(22)	1.111(22)	1.090(22)	1.115(22)
C9-H92	1.091(22)	1.110(22)	1.089(22)	1.114(22)
C9-H93	1.092(22)	1.110(22)	1.090(22)	1.114(21)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
C1-C2	1.5458(5)	1.5400(4)	1.5395(5)	1.5337(5)	1.549(3)
C1-C6	1.5472(4)	1.5406(4)	1.5398(4)	1.5326(4)	1.545(3)
C1-C7	1.5580(5)	1.5237(4)	1.5477(5)	1.5484(4)	1.557(3)

C1-H11	1.0879(5)	1.1089(6)	1.0854(7)	1.1086(4)	1.002(9)
C2-C3	1.5382(4)	1.5294(4)	1.5318(5)	1.5296(4)	1.539(3)
C2-H21	1.0858(4)	1.1026(4)	1.0832(4)	1.1038(5)	1.005(9)
C2-H22	1.0841(4)	1.1014(4)	1.0815(4)	1.1011(5)	1.000(9)
C3-C4	1.5347(4)	1.5239(5)	1.5275(4)	1.5227(5)	1.537(3)
C3-H31	1.0844(4)	1.1026(5)	1.0820(5)	1.1038(5)	0.997(9)
C3-H32	1.0836(4)	1.1026(4)	1.0809(4)	1.1016(5)	1.001(9)
C4-C5	1.5366(4)	1.5252(4)	1.5293(4)	1.5244(4)	1.538(3)
C4-H41	1.0843(3)	1.1035(4)	1.0817(3)	1.1056(5)	1.001(9)
C4-H42	1.0840(4)	1.1027(5)	1.0815(4)	1.1012(5)	1.000(9)
C5-C6	1.5385(5)	1.5305(4)	1.5316(4)	1.5302(4)	1.539(3)
C5-H51	1.0853(4)	1.1027(4)	1.0826(4)	1.1023(5)	1.000(9)
C5-H52	1.0848(4)	1.1028(4)	1.0826(5)	1.1039(4)	1.001(9)
C6-H61	1.0840(4)	1.1019(4)	1.0814(4)	1.1012(6)	1.001(9)
C6-H62	1.0847(4)	1.1015(5)	1.0822(5)	1.1031(5)	1.004(9)
C7-C8	1.5425(5)	1.5334(4)	1.5330(5)	1.5302(4)	1.540(3)
C7-C9	1.5384(4)	1.5313(4)	1.5292(4)	1.5304(5)	1.541(3)
C7-H71	1.0878(5)	1.1098(4)	1.0857(8)	1.1098(5)	1.003(9)
C8-H81	1.0796(105)	1.0949(359)	1.0743(274)	1.0180(1547)	0.999(9)
C8-H82	1.0780(104)	1.0912(360)	1.0734(273)	1.0140(1538)	1.004(9)
C8-H83	1.0791(103)	1.0918(351)	1.0740(275)	1.0138(1540)	1.002(9)
C9-H91	1.0785(347)	1.0963(272)	1.0783(5)	1.0749(801)	1.004(9)

C9-H92	1.0754(344)	1.0928(273)	1.0756(4)	1.0698(792)	1.002(9)
C9-H93	1.0769(348)	1.0929(274)	1.0768(5)	1.0704(793)	0.997(9)

Ueq

atom	gaff	charmm	opls	mm3	experiment
C1	0.0131(3)	0.0165(4)	0.0129(2)	0.0309(4)	0.0240(9)
C2	0.0165(3)	0.0216(4)	0.0163(3)	0.0397(5)	0.0271(9)
C3	0.0194(3)	0.0251(5)	0.0193(3)	0.0465(6)	0.0310(9)
C4	0.0211(3)	0.0262(5)	0.0209(3)	0.0486(6)	0.0338(10)
C5	0.0211(3)	0.0270(4)	0.0209(3)	0.0490(6)	0.0341(10)
C6	0.0174(3)	0.0223(4)	0.0174(3)	0.0404(5)	0.0296(10)
C7	0.0161(3)	0.0209(4)	0.0156(2)	0.0377(4)	0.0271(9)
C8	0.0216(3)	0.0298(5)	0.0212(3)	0.0528(6)	0.0346(11)
C9	0.0249(3)	0.0320(4)	0.0242(3)	0.0552(6)	0.0358(11)
H11	0.0186(3)	0.0237(4)	0.0186(3)	0.0419(5)	0.044(2)
H21	0.0264(3)	0.0357(5)	0.0267(3)	0.0599(8)	0.044(2)
H22	0.0243(3)	0.0321(5)	0.0247(3)	0.0551(7)	0.044(2)
H31	0.0304(4)	0.0408(6)	0.0311(3)	0.0711(8)	0.044(2)
H32	0.0275(3)	0.0355(5)	0.0281(3)	0.0612(7)	0.044(2)
H41	0.0332(3)	0.0412(6)	0.0336(3)	0.0707(8)	0.044(2)
H42	0.0294(3)	0.0370(5)	0.0297(3)	0.0651(7)	0.044(2)
H51	0.0299(3)	0.0385(5)	0.0302(3)	0.0645(7)	0.044(2)

H52	0.0332(4)	0.0444(5)	0.0335(4)	0.0754(9)	0.044(2)
H61	0.0248(3)	0.0321(5)	0.0255(3)	0.0549(6)	0.044(2)
H62	0.0279(3)	0.0366(5)	0.0285(3)	0.0608(6)	0.044(2)
H71	0.0220(3)	0.0289(4)	0.0218(3)	0.0490(6)	0.044(2)
H81	0.0374(66)	0.0495(208)	0.0388(165)	0.126(88)	0.043(3)
H82	0.0321(68)	0.0451(211)	0.0338(173)	0.121(91)	0.043(3)
H83	0.0301(75)	0.0436(211)	0.0314(174)	0.119(90)	0.043(3)
H91	0.0388(202)	0.0491(171)	0.0371(4)	0.092(49)	0.043(3)
H92	0.0403(200)	0.0492(169)	0.0382(4)	0.093(49)	0.043(3)
H93	0.0375(203)	0.0472(169)	0.0359(4)	0.090(49)	0.043(3)

Table S5. Decane 150 K

supercell 6 x 5 x 2, 25.0446 x 23.6195 x 27.0132 A, 60 molecules, 1920 atoms

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	4.1636(57)	4.1754(63)	4.1397(56)	4.2937(42)	4.1741(4)
b, Å	4.7120(64)	4.7254(71)	4.6850(63)	4.8593(48)	4.7239(6)
c, Å	13.4726(183)	13.5109(202)	13.3953(180)	13.8938(137)	13.5066(15)
α, °	86.095	86.095	86.095	85.974	85.9740(10)
β, °	81.463	81.463	81.463	81.463	81.463(7)
γ, °	75.545	75.545	75.545	74.652	74.652(6)

Average bond lengths

bond	gaff	charmm	opls	mm3
C1-C2	1.5390(220)	1.5295(223)	1.5318(233)	1.5370(225)
C1-H1A	1.092(22)	1.112(22)	1.090(22)	1.115(22)
C1-H1B	1.092(22)	1.111(22)	1.090(22)	1.115(22)
C1-H1C	1.092(22)	1.111(22)	1.090(22)	1.115(22)
C2-C3	1.5426(218)	1.5326(227)	1.5338(232)	1.5395(226)
C2-H2A	1.092(22)	1.114(22)	1.091(22)	1.116(22)
C2-H2B	1.092(22)	1.114(22)	1.091(22)	1.116(22)
C3-C4	1.5428(218)	1.5333(227)	1.5345(232)	1.5400(227)
C3-H3A	1.093(22)	1.114(22)	1.091(22)	1.116(22)
C3-H3B	1.093(22)	1.113(22)	1.091(22)	1.116(22)

C4-C5	1.5427(218)	1.5332(226)	1.5343(232)	1.5398(227)
C4-H4A	1.093(22)	1.113(22)	1.091(22)	1.116(22)
C4-H4B	1.093(22)	1.113(22)	1.091(22)	1.116(22)
C5-C5	1.5427(218)	1.5331(226)	1.5343(232)	1.5399(225)
C5-H5A	1.093(22)	1.113(22)	1.091(22)	1.116(22)
C5-H5B	1.093(22)	1.113(22)	1.091(22)	1.116(22)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
C1-C2	1.5305(4)	1.5185(4)	1.5224(5)	1.5235(5)	1.5232(18)
C1-H1A	1.0719(5)	1.0877(6)	1.0678(4)	-[2]	0.976(18)
C1-H1B	1.0719(5)	1.0871(6)	1.0677(5)	-	0.946(18)
C1-H1C	1.0762(5)	1.0927(6)	1.0726(5)	-	1.01(2)
C2-C3	1.5360(4)	1.5244(4)	1.5264(4)	1.5293(5)	1.5242(15)
C2-H2A	1.0809(5)	1.0999(4)	1.0775(5)	1.0987(4)	0.994(16)
C2-H2B	1.0808(5)	1.0997(4)	1.0773(5)	1.0993(5)	0.963(16)
C3-C4	1.5376(6)	1.5267(5)	1.5285(4)	1.5321(4)	1.5233(16)
C3-H3A	1.0829(4)	1.1015(4)	1.0794(4)	1.1023(4)	0.979(16)
C3-H3B	1.0831(4)	1.1012(4)	1.0796(4)	1.1017(5)	0.974(15)
C4-C5	1.5378(5)	1.5270(5)	1.5287(4)	1.5323(5)	1.5257(15)
C4-H4A	1.0840(4)	1.1024(4)	1.0805(5)	1.1035(5)	0.972(15)
C4-H4B	1.0838(4)	1.1024(4)	1.0809(4)	1.1036(4)	0.976(16)

2 trajectory not corrected for methyl rotation

C5-C5	1.5378(6)	1.5272(5)	1.5286(4)	1.5328(4)	1.523(2)
C5-H5A	1.0840(4)	1.1026(4)	1.0805(4)	1.1041(4)	0.974(16)
C5-H5B	1.0841(4)	1.1028(4)	1.0808(4)	1.1040(4)	0.988(16)

Ueq

atom	gaff	charmm	opls	mm3	experiment
C1	0.0244(3)	0.0338(4)	0.0251(3)	0.0535(6)	0.0378(5)
H1A	0.0398(4)	0.0536(5)	0.0427(5)	0.240[3]	0.047(4)
H1B	0.0429(4)	0.0568(5)	0.0455(4)	0.242	0.048(4)
H1C	0.0404(4)	0.0545(6)	0.0421(5)	0.242	0.058(5)
C2	0.0187(3)	0.0249(4)	0.0195(3)	0.0412(5)	0.0314(4)
H2A	0.0303(4)	0.0396(5)	0.0330(5)	0.0589(7)	0.041(4)
H2B	0.0317(4)	0.0410(5)	0.0344(4)	0.0611(7)	0.039(4)
C3	0.0156(3)	0.0210(3)	0.0164(2)	0.0347(4)	0.0269(4)
H3A	0.0248(4)	0.0329(4)	0.0272(3)	0.0485(5)	0.032(3)
H3B	0.0254(3)	0.0335(4)	0.0277(3)	0.0495(5)	0.031(3)
C4	0.0151(3)	0.0198(3)	0.0159(3)	0.0330(4)	0.0269(4)
H4A	0.0239(3)	0.0309(4)	0.0262(4)	0.0461(5)	0.035(4)
H4B	0.0242(3)	0.0313(4)	0.0266(4)	0.0465(5)	0.032(3)
C5	0.0147(3)	0.0194(3)	0.0156(2)	0.0321(4)	0.0265(4)
H5A	0.0233(3)	0.0303(4)	0.0257(3)	0.0448(4)	0.031(3)
H5B	0.0233(3)	0.0302(4)	0.0257(3)	0.0448(5)	0.036(4)

3 uncorrected for motion

Table S6. Imidazole 103 K

supercell 4 x 5 x 3, 30.276 x 26.83 x 29.355 A, 240 molecules, 2160 atoms

Unit cell parameters

parameter	gaff	charmm[4]	opls	mm3	experiment
a, Å	7.529(6)	6.84	7.615(6)	7.783(16)	7.569(1)
b, Å	5.338(5)	5.28	5.347(4)	5.518(11)	5.366(1)
c, Å	9.734(8)	9.62	9.751(8)	10.062(20)	9.785(2)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	119.08	105.85	119.08	119.08	119.08
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
N1-C2	1.368(15)	1.352(15)	1.332(14)	1.271(13)
N1-C5	1.372(15)	1.377(15)	1.387(15)	1.269(13)
C2-N3	1.340(14)	1.320(15)	1.329(14)	1.267(13)
N3-C4	1.376(15)	1.387(15)	1.397(15)	1.270(14)
C4-C5	1.363(14)	1.356(15)	1.374(14)	1.339(14)
N1-H1	1.020(16)	1.014(15)	1.023(16)	1.035(15)
C2-H2	1.079(17)	1.093(17)	1.081(17)	1.100(15)
C4-H4	1.082(18)	1.083(17)	1.080(17)	1.101(16)
C5-H5	1.083(18)	1.080(17)	1.080(17)	1.098(16)

4 phase transition, all data refers to the new polymorph

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
N1-C2	1.3604(4)	1.3410(5)	1.3254(4)	-	1.358(1)
N1-C5	1.3645(4)	1.3691(8)	1.3800(4)	-	1.381(1)
C2-N3	1.3331(4)	1.3126(5)	1.3224(4)	-	1.333(1)
N3-C4	1.3687(4)	1.3770(6)	1.3892(4)	-	1.389(1)
C4-C5	1.3557(4)	1.3462(5)	1.3665(5)	-	1.378(1)
N1-H1	1.0142(4)	1.0072(4)	1.0170(4)	-	1.053(2)
C2-H2	1.0718(4)	1.0840(6)	1.0735(4)	-	1.087(2)
C4-H4	1.0753(4)	1.0736(4)	1.0731(4)	-	1.086(2)
C5-H5	1.0750(4)	1.0688(6)	1.0729(4)	-	1.087(2)

Ueq

atom	gaff	charmm	opls	mm3	experiment
N1	0.0143(2)	0.0237(4)	0.0127(2)	-	0.0160(2)
H1	0.0230(2)	0.0320(5)	0.0202(2)	-	0.0298(6)
C2	0.0161(2)	0.0226(4)	0.0142(2)	-	0.0172(2)
H2	0.0293(3)	0.0371(7)	0.0266(2)	-	0.0432(6)
N3	0.0175(2)	0.0251(5)	0.0163(2)	-	0.0187(2)
C4	0.0165(2)	0.0246(4)	0.0154(2)	-	0.0197(2)
H4	0.0304(3)	0.0408(7)	0.0293(3)	-	0.0468(7)
C5	0.0158(2)	0.0270(5)	0.0143(2)	-	0.0187(2)
H5	0.0296(3)	0.0482(8)	0.0272(2)	-	0.0450(7)

Table S7. Diaminoheptane 130 K

supercell 1 x 4 x 4, 22.813 x 25.46 x 23.004 A, 64 mol, 1728 atoms

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	22.271(26)	22.522(24)	22.243(28)	23.204(7)	22.813(4)
b, Å	6.2137(74)	6.2839(66)	6.2059(77)	6.474(2)	6.3654(14)
c, Å	5.6143(67)	5.6777(59)	5.6073(70)	5.850(2)	5.7511(11)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
N C1	1.4728(200)	1.4695(210)	1.4515(18)	1.4708(191)
N H1	1.032(19)	1.012(18)	1.026(18)	1.022(18)
N H2	1.027(19)	1.006(18)	1.020(18)	1.022(18)
C1 C2	1.5367(203)	1.5303(222)	1.5297(216)	1.5353(211)
C1 H1A	1.094(20)	1.086(20)	1.091(20)	1.114(20)
C1 H1B	1.094(20)	1.087(20)	1.091(20)	1.114(20)
C2 C3	1.5439(202)	1.5396(210)	1.5370(215)	1.5383(212)
C2 H2A	1.092(20)	1.112(20)	1.090(20)	1.115(20)
C2 H2B	1.091(20)	1.112(20)	1.090(20)	1.115(20)
C3 C4	1.5436(202)	1.5350(210)	1.5361(215)	1.5400(211)

C3 H3A	1.092(20)	1.113(20)	1.090(20)	1.116(20)
C3 H3B	1.092(20)	1.114(20)	1.091(20)	1.115(20)
C4 C3	1.5436(202)	1.5355(210)	1.5361(215)	1.5400(211)
C4 H4A	1.092(20)	1.112(20)	1.090(20)	1.116(20)
C4 H4B	1.092(20)	1.113(20)	1.089(20)	1.115(20)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
N C1	1.4682(5)	1.4642(4)	1.4469(5)	1.4636(4)	1.4686(9)
N H1	1.0248(4)	1.0024(4)	1.0184(5)	1.0073(5)	0.90(2)
N H2	1.0197(4)	0.9959(5)	1.0114(4)	1.0071(5)	0.841(12)
C1 C2	1.5331(4)	1.5257(5)	1.5257(4)	1.5294(5)	1.5272(11)
C1 H1A	1.0876(5)	1.0783(4)	1.0841(3)	1.1041(5)	0.980(11)
C1 H1B	1.0880(4)	1.0791(5)	1.0846(3)	1.1044(5)	0.93(2)
C2 C3	1.5409(4)	1.5357(4)	1.5336(4)	1.5333(5)	1.5270(10)
C2 H2A	1.0864(5)	1.1046(4)	1.0838(5)	1.1068(4)	0.97(2)
C2 H2B	1.0854(5)	1.1049(4)	1.0828(5)	1.1061(5)	0.961(10)
C3 C4	1.5409(4)	1.5312(5)	1.5328(4)	1.5353(5)	1.5272(9)
C3 H3A	1.0866(3)	1.1061(4)	1.0841(4)	1.1073(4)	0.989(11)
C3 H3B	1.0874(3)	1.1074(5)	1.0847(4)	1.1077(5)	0.97(2)
C4 C3	1.5408(5)	1.5316(6)	1.5329(4)	1.5353(5)	1.5272(9)
C4 H4A	1.0869(5)	1.1055(4)	1.0844(4)	1.1075(4)	0.98(3)
C4 H4B	1.0862(4)	1.1060(3)	1.0838(5)	1.1074(4)	0.952(13)

Ueq

atom	gaff	charmm	opls	mm3	experiment
N	0.0113(1)	0.0150(2)	0.0124(2)	0.0217(2)	0.0218(2)
H1	0.0156(1)	0.0202(2)	0.0163(2)	0.0318(3)	0.030(3)
H2	0.0180(2)	0.0243(2)	0.0195(2)	0.0336(2)	0.036(3)
C1	0.0095(1)	0.0127(2)	0.0109(1)	0.0172(2)	0.0202(2)
H1A	0.0160(1)	0.0200(2)	0.0177(2)	0.0278(2)	0.021(3)
H1B	0.0159(1)	0.0202(2)	0.0177(2)	0.0273(2)	0.027(3)
C2	0.0088(1)	0.0121(1)	0.0103(1)	0.0160(2)	0.0199(2)
H2A	0.0140(1)	0.0190(2)	0.0162(2)	0.0252(2)	0.024(3)
H2B	0.0140(1)	0.0188(2)	0.0158(2)	0.0245(2)	0.018(3)
C3	0.0090(09)	0.0128(2)	0.0109(1)	0.0163(2)	0.0215(3)
H3A	0.0139(1)	0.0201(2)	0.0168(1)	0.0253(2)	0.023(3)
H3B	0.0136(1)	0.0196(2)	0.0164(1)	0.0245(2)	0.033(4)
C4	0.0090(09)	0.0128(2)	0.0109(1)	0.0165(2)	0.0210(3)
H4A	0.0139(1)	0.0199(2)	0.0168(1)	0.0253(2)	0.034(5)
H4B	0.0134(1)	0.0191(2)	0.0161(1)	0.0244(2)	0.016(4)

Table S8. Diaminoheptane 213 K

supercell 1 x 4 x 4, 22.806 x 25.800 x 23.252, 64 mol, 1728 atoms

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	22.246(32)	22.517(31)	22.234(34)	23.239(14)	22.806(7)
b, Å	6.292(9)	6.368(9)	6.288(10)	6.573(4)	6.450(2)
c, Å	5.670(8)	5.739(8)	5.667(9)	5.923(4)	5.813(2)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
N1 C2	1.473(26)	1.469(27)	1.451(24)	1.472(25)
N1 H11	1.027(24)	1.006(23)	1.019(23)	1.022(22)
N1 H12	1.032(24)	1.011(23)	1.025(23)	1.022(23)
C2 C3	1.537(26)	1.531(28)	1.530(28)	1.537(27)
C2 H2A	1.095(26)	1.087(25)	1.092(26)	1.116(26)
C2 H2B	1.094(26)	1.086(25)	1.092(26)	1.116(26)
C3 C4	1.544(26)	1.540(27)	1.537(28)	1.540(27)
C3 H3A	1.091(26)	1.112(26)	1.090(26)	1.116(26)
C3 H3B	1.092(26)	1.112(26)	1.090(26)	1.117(27)

C4 C5	1.544(26)	1.535(27)	1.537(28)	1.542(27)
C4 H4A	1.093(26)	1.115(26)	1.091(26)	1.117(26)
C4 H4B	1.092(26)	1.114(26)	1.091(26)	1.117(26)
C5 C4	1.544(26)	1.536(27)	1.537(28)	1.542(27)
C5 H5A	1.092(26)	1.113(26)	1.091(26)	1.117(26)
C5 H5B	1.092(26)	1.113(26)	1.091(26)	1.117(26)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
N1 C2	1.4645(5)	1.4598(4)	1.4431(5)	1.4579(21)	1.448(4)
N1 H11	1.01378(4)	0.9872(5)[5]	1.0049(5)	-[6]	0.85(3)
N1 H12	1.0192(5)	0.9940(5)	1.0122(5)	-	0.94(5)
C2 C3	1.5305(5)	1.5222(4)	1.5229(5)	1.5256(7)	1.541(4)
C2 H2A	1.0836(5)	1.0734(5)	1.0797(4)	1.0968(20)	0.98
C2 H2B	1.0831(4)	1.0725(5)	1.0790(3)	1.0963(19)	0.98
C3 C4	1.5387(5)	1.5327(4)	1.5314(4)	1.5306(6)	1.512(4)
C3 H3A	1.0820(4)	1.0998(4)	1.0789(5)	1.1004(5)	0.98
C3 H3B	1.0830(5)	1.0996(5)	1.0798(4)	1.1011(6)	0.98
C4 C5	1.5392(5)	1.5283(5)	1.5308(5)	1.5328(5)	1.532(4)
C4 H4A	1.0842(4)	1.1022(4)	1.0807(5)	1.1024(5)	0.98
C4 H4B	1.0834(5)	1.1010(5)	1.0802(5)	1.1020(5)	0.98

5 N-H bond lengths are not corrected for motion
6 trajectory not corrected for considerable motion

C5 C4	1.5391(6)	1.5287(5)	1.5308(4)	1.5328(6)	1.533(4)
C5 H5A	1.0839(4)	1.1006(5)	1.0805(4)	1.1026(5)	0.98
C5 H5B	1.0833(5)	1.1012(4)	1.0799(5)	1.1022(5)	0.98

Ueq

atom	gaff	charmm	opls	mm3	experiment
N1	0.0211(2)	0.0290(4)	0.0234(2)	0.0477(41)	0.0523(11)
C2	0.0177(2)	0.0244(3)	0.0203(2)	0.0367(22)	0.0520(12)
H2A	0.0291(3)	0.0381(4)	0.0325(3)	0.0562(36)	0.062
H2B	0.0292(3)	0.0378(4)	0.0325(3)	0.0572(37)	0.062
C3	0.0161(2)	0.0229(3)	0.0190(2)	0.0334(14)	0.0480(13)
H3A	0.0249(2)	0.0350(4)	0.0289(2)	0.0492(16)	0.058
H3B	0.0255(2)	0.0357(4)	0.0295(2)	0.0502(21)	0.058
C4	0.0164(2)	0.0242(3)	0.0199(2)	0.0330(10)	0.0536(15)
H4A	0.0247(2)	0.0364(4)	0.0297(3)	0.0483(12)	0.064
H4B	0.0254(2)	0.0373(4)	0.0305(3)	0.0500(12)	0.064
C5	0.0164(2)	0.0241(3)	0.0200(2)	0.0331(10)	0.049(2)
H5A	0.0252(2)	0.0369(3)	0.0305(3)	0.050(13)	0.059
H5B	0.0245(2)	0.0355(3)	0.0292(3)	0.0480(12)	0.059
H11	0.0329(3)	0.0459(5)	0.0359(3)	0.185(77)	0.065(12)
H12	0.0286(3)	0.0384(4)	0.0304(3)	0.194(88)	0.076(15)

Table S9. Alanine 60 K

supercell 4 x 2 x 4 which is 23.768 x 24.522 x 23.140 A, 128 molecules, 1664 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	5.971(4)	5.828(5)	5.821(5)	5.271(34)	5.942(3)
b, Å	12.320(8)	12.026(10)	12.011(10)	10.877(70)	12.261(5)
c, Å	5.813(4)	5.674(5)	5.667(5)	5.132(33)	5.785(3)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
N1-H1	1.054(13)	1.053(13)	1.035(13)	1.245(75)
N1-H4	1.048(13)	1.055(13)	1.025(12)	1.262(41)
N1-H6	1.047(13)	1.050(13)	1.029(13)	1.139(49)
N1-C2	1.5467(140)	1.4798(154)	1.4781(126)	1.424(15)
C2-H2	1.093(14)	1.078(14)	1.087(14)	1.101(10)
C2-C3	1.5383(139)	1.5411(148)	1.5330(146)	1.510(14)
C3-H3	1.092(14)	1.111(14)	1.089(14)	1.099(10)
C3-H5	1.093(14)	1.111(14)	1.090(14)	1.098(9)
C3-H7	1.091(14)	1.110(14)	1.089(14)	1.097(9)
C1-C2	1.5490(132)	1.5492(145)	1.5543(133)	1.521(15)

C1-O1	1.2140(96)	1.2579(101)	1.2481(96)	1.245(12)
C1-O2	1.2159(96)	1.2614(101)	1.2537(96)	1.244(12)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
N1-H1	1.0521(4)	1.0510(4)	1.0330(4)	-	1.036(4)
N1-H4	1.0458(3)	1.0533(4)	1.0234(4)	-	1.050(4)
N1-H6	1.0446(4)	1.0477(4)	1.0268(4)	-	1.038(3)
N1-C2	1.5453(4)	1.4787(4)	1.4771(5)	-	1.4906(14)
C2-H2	1.0905(5)	1.0765(4)	1.0848(4)	-	1.099(4)
C2-C3	1.5361(4)	1.5396(4)	1.5316(5)	-	1.5249(15)
C3-H3	1.0884(4)	1.1076(5)	1.0862(4)	-	1.086(6)
C3-H5	1.0900(5)	1.1077(5)	1.0875(4)	-	1.092(5)
C3-H7	1.0879(4)	1.1072(4)	1.0862(4)	-	1.093(5)
C1-C2	1.5478(4)	1.5485(5)	1.5535(5)	-	1.5357(16)
C1-O1	1.2103(4)	1.2566(4)	1.2458(4)	-	1.2487(16)
C1-O2	1.2120(4)	1.2600(4)	1.2517(5)	-	1.2649(19)

Ueq

atom	gaff	charmm	opls	mm3	experiment
N1	0.00356(6)	0.00211(3)	0.00204(3)	-	0.00802(11)
H1	0.00499(7)	0.00351(5)	0.00324(4)	-	0.0213(6)

H4	0.00542(7)	0.00341(4)	0.00335(3)	-	0.0196(5)
H6	0.00528(8)	0.00372(4)	0.00325(4)	-	0.0201(5)
C2	0.00337(6)	0.00185(3)	0.00181(3)	-	0.00709(14)
H2	0.00558(7)	0.00328(3)	0.00339(3)	-	0.0201(5)
C3	0.00601(7)	0.00330(3)	0.00336(3)	-	0.01016(17)
H5	0.00898(9)	0.00614(5)	0.00601(4)	-	0.0273(8)
H3	0.00940(9)	0.00634(5)	0.00587(5)	-	0.0295(9)
H7	0.00975(9)	0.00623(5)	0.00626(5)	-	0.0280(8)
C1	0.00356(6)	0.00183(4)	0.00178(4)	-	0.00686(14)
O1	0.00499(7)	0.00275(5)	0.00382(5)	-	0.00942(18)
O2	0.00542(7)	0.00299(5)	0.00314(4)	-	0.01012(19)

Table S10. Alanine 295 K

supercell 4 x 2 x 4, 24.172 x 24.674 x 23.136 A, 128 molecules, 1664 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	6.093(8)	5.931(7)	5.924(7)	5.835(107)	6.043(3)
b, Å	12.439(17)	12.109(15)	12.093(15)	11.913(218)	12.337(5)
c, Å	5.832(8)	5.677(7)	5.670(7)	5.585(102)	5.784(3)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
N1-H1	1.047(29)	1.050(28)	1.029(28)	1.153(63)
N1-H4	1.049(29)	1.055(28)	1.025(27)	1.239(64)
N1-H6	1.056(28)	1.053(28)	1.034(28)	1.160(64)
N1-C2	1.548(31)	1.482(34)	1.480(28)	1.466(39)
C2-H2	1.094(30)	1.080(30)	1.089(30)	1.118(30)
C2-C3	1.539(31)	1.543(33)	1.535(32)	1.531(32)
C3-H3	1.092(30)	1.111(30)	1.090(30)	1.113(30)
C3-H5	1.093(30)	1.112(30)	1.091(30)	1.112(30)
C3-H7	1.093(30)	1.112(30)	1.090(30)	1.113(30)
C1-C2	1.552(29)	1.551(32)	1.556(30)	1.576(39)

C1-O1	1.214(21)	1.261(22)	1.254(21)	1.269(26)
C1-O2	1.217(21)	1.259(22)	1.249(21)	1.265(24)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
N1-H1	1.0346(5)	1.0384(5)	1.0196(4)	-	1.031(6)
N1-H4	1.0378(5)	1.0455(5)	1.0159(5)	-	1.071(8)
N1-H6	1.0439(4)	1.0421(5)	1.0244(4)	-	1.037(7)
N1-C2	1.5411(4)	1.4771(4)	1.4746(5)	-	1.491(3)
C2-H2	1.0833(7)	1.0720(5)	1.0797(4)	-	1.099(7)
C2-C3	1.5280(5)	1.5357(5)	1.5273(4)	-	1.525(4)
C3-H3	1.0748(6)	1.0952(5)	1.0744(5)	-	1.114(11)
C3-H5	1.0770(6)	1.0963(4)	1.0763(4)	-	1.095(11)
C3-H7	1.0749(6)	1.0947(5)	1.0744(4)	-	1.093(12)
C1-C2	1.5451(5)	1.5473(5)	1.5520(4)	-	1.532(3)
C1-O1	1.1966(5)	1.2542(5)	1.2431(4)	-	1.245(4)
C1-O2	1.1984(5)	1.2517(4)	1.2370(4)	-	1.259(4)

Ueq

atom	gaff	charmm	opls	mm3	experiment
N1	0.0193(3)	0.0117(2)	0.0110(1)	-	0.0279(3)
H1	0.0283(4)	0.0206(2)	0.0174(2)	-	0.0430(13)
H4	0.0291(3)	0.0185(2)	0.0181(2)	-	0.0424(12)

H6	0.0268(4)	0.0194(2)	0.0175(2)	-	0.0438(13)
C2	0.0179(3)	0.0100(2)	0.0097(1)	-	0.0254(4)
H2	0.0289(4)	0.0173(2)	0.0177(2)	-	0.0445(13)
C3	0.0313(4)	0.0174(2)	0.0177(2)	-	0.0364(6)
H5	0.0519(5)	0.0326(3)	0.0330(3)	-	0.066(3)
H3	0.0481(6)	0.0319(2)	0.0298(2)	-	0.063(2)
H7	0.0470(5)	0.0317(3)	0.0312(2)	-	0.065(3)
C1	0.0192(4)	0.0101(2)	0.0097(2)	-	0.0250(4)
O1	0.0305(5)	0.0165(2)	0.0169(2)	-	0.0354(7)
O2	0.0311(5)	0.0153(2)	0.0202(3)	-	0.0369(7)

Table S11. L-alanyl-glycyl-L-alanine 293 K

supercell 6 x 2 x 2, 28.482 x 28.798 x 30.382 A, 96 molecules, 2880 at

Unit cell parameters

parameter	gaff	charmm	opls	mm3	experiment
a, Å	4.866(11)	4.753(5)	4.765(5)	4.512(8)	4.747(7)
b, Å	14.760(34)	14.418(14)	14.452(14)	13.686(24)	14.399(2)
c, Å	15.572(34)	15.211(15)	15.247(15)	14.439(26)	15.191(2)
α, °	90.00	90.00	90.00	90.00	90.00
β, °	90.00	90.00	90.00	90.00	90.00
γ, °	90.00	90.00	90.00	90.00.	90.00

Average bond lengths

bond	gaff	charmm	opls	mm3
N1 C1A	1.535(31)	1.489(34)	1.477(28)	1.504(32)
C1A C1B	1.537(31)	1.547(33)	1.539(32)	1.522(32)
C1A C1'	1.554(29)	1.518(33)	1.548(29)	1.500(32)
C1A H1A	1.093(30)	1.081(30)	1.089(30)	1.115(30)
C1B H	1.092(30)	1.112(30)	1.091(30)	1.113(30)
C1' O1'	1.218(21)	1.232(22)	1.231(23)	1.214(21)
C1' N2	1.347(25)	1.347(28)	1.338(24)	1.380(25)
N2 C2A	1.489(29)	1.450(30)	1.465(29)	1.453(28)
C2A C2'	1.525(30)	1.502(34)	1.540(30)	1.525(32)
C2A H	1.093(30)	1.080(30)	1.088(30)	1.114(30)

C2' N3	1.344(25)	1.341(28)	1.339(24)	1.382(25)
C2' O2'	1.215(21)	1.230(22)	1.233(23)	1.209(20)
N3 C3A	1.493(29)	1.447(30)	1.479(29)	1.446(28)
C3A C3B	1.545(31)	1.537(33)	1.534(32)	1.515(31)
C3A C3'	1.540(29)	1.556(32)	1.564(29)	1.572(31)
C3A H3A	1.093(30)	1.082(30)	1.089(30)	1.110(29)
C3B H	1.093(30)	1.110(30)	1.089(30)	1.112(30)
C3' O3	1.217(21)	1.257(22)	1.247(21)	1.272(24)
C3' O3'	1.216(21)	1.262(22)	1.259(21)	1.278(24)
N1 H	1.043(29)	1.051(28)	1.022(28)	1.162(54)
N2 HN2	1.016(28)	1.015(27)	1.033(28)	1.047(27)
N3 HN3	1.017(28)	1.001(27)	1.015(27)	1.050(28)

Bond lengths from average positions

bond	gaff	charmm	opls	mm3	experiment
N1 C1A	-	1.4758(4)	1.4656(5)	-	1.485(2)
C1A C1B	-	1.5245(6)	1.5177(5)	-	1.513(3)
C1A C1'	-	1.5126(6)	1.5410(5)	-	1.521(2)
C1A H1A	-	1.0632(6)	1.0702(5)	-	0.98
C1B H	-	0.7740(0.1836)[7]	0.4375(421)	-	0.96
C1' O1'	-	1.2225(5)	1.2216(5)	-	1.229(2)
C1' N2	-	1.3393(4)	1.3298(4)	-	1.325(2)

7 uncorrected for motion for both CHARMM and OPLS

N2 C2A	-	1.4433(6)	1.4582(5)	-	1.442(2)
C2A C2'	-	1.4945(4)	1.5325(5)	-	1.518(2)
C2A H	-	1.0657(5)	1.0700(7)	-	0.97
C2' N3	-	1.3315(5)	1.3311(5)	-	1.333(2)
C2' O2'	-	1.2169(5)	1.2212(5)	-	1.234(3)
N3 C3A	-	1.4415(4)	1.4732(4)	-	1.455(2)
C3A C3B	-	1.5261(5)	1.5236(5)	-	1.516(3)
C3A C3'	-	1.5478(4)	1.5561(5)	-	1.541(2)
C3A H3A	-	1.0736(4)	1.0787(5)	-	0.98
C3B H	-	0.7530(0.1899)[8]	0.4814(736)	-	0.96
C3' O3	-	1.2410(4)	1.2298(9)	-	1.231(2)
C3' O3'	-	1.2503(5)	1.2469(7)	-	1.260(2)
N1 H	-	1.0347(102)	0.9947(613)	-	0.89
N2 HN2	-	1.0041(4)	1.0216(7)	-	0.86
N3 HN3	-	0.9882(5)	1.0001(4)	-	0.86

Ueq

atom	gaff	charmm	opls	mm3	experiment
N1	-	0.0273(5)	0.0276(7)	-	0.0315(4)
H1N1	-	0.0508(6)	0.0546	-	0.059(8)
H2N1	-	0.0351(5)	0.0437	-	0.053(8)
H3N1	-	0.0415(5)	0.0464	-	0.067(9)

8 uncorrected for motion for both CHARMM and OPLS

C1A	-	0.0185(2)	0.0183(3)	-	0.0265(4)
H1A	-	0.0351(3)	0.0363(5)	-	0.029(5)
C1B	-	0.0436(4)	0.0396(4)	-	0.0551(8)
H11B	-	0.2536[9]	0.3814	-	0.072(9)
H21B	-	0.2578	0.3824	-	0.063(9)
H31B	-	0.2588	0.03819	-	0.085(12)
C1'	-	0.0170(2)	0.0177(3)	-	0.0216(3)
O1'	-	0.0296(3)	0.0308(4)	-	0.0321(3)
N2	-	0.0183(2)	0.0196(2)	-	0.0267(3)
HN2	-	0.0271(3)	0.0260(2)	-	0.029(5)
C2A	-	0.0215(2)	0.0235(3)	-	0.0257(4)
H12A	-	0.0368(3)	0.0455(5)	-	0.037(6)
H22A	-	0.0385(4)	0.0445(4)	-	0.030(5)
C2'	-	0.0187(2)	0.0184(2)	-	0.0241(4)
O2'	-	0.0402(5)	0.0347(5)	-	0.0411(4)
N3	-	0.0148(2)	0.0159(2)	-	0.0239(3)
HN3	-	0.0248(2)	0.0271(2)	-	0.054(8)
C3A	-	0.0146(2)	0.0142(2)	-	0.0240(4)
H3A	-	0.0230(2)	0.0238(2)	-	0.026(5)
C3B	-	0.0286(3)	0.0267(3)	-	0.0434(6)
H13B	-	0.246	0.349	-	0.089(11)

9 H11B, H21B, H31B and H13B, H22B, H33B are uncorrected for motion for both CHARMM and OPLS

H23B	-	0.245	0.349	-	0.050(7)
H33B	-	0.243	0.348	-	0.075(10)
C3'	-	0.0175(2)	0.0170(2)	-	0.0310(4)
O3'	-	0.0270(3)	0.0263(5)	-	0.0395(4)
O3	-	0.0366(4)	0.0364(11)	-	0.0641(6)

Table S12. Effect of length of simulation on the simulation results.

AGA 64 mol (1920 atoms), cutoff 12.

geometry						Ueq					
parameter	0.5 ns	1 ns	2 ns	10 ns	exp	atom	0.5 ns	1 ns	2 ns	10 ns	exp
a, Å	4.753(6)	4.753(6)	4.753(6)	4.753(6)	4.747(7)	N1	0.0272(8)	0.0272(7)	0.0272(8)	0.0272(7)	0.0315(4)
b, Å	14.418(18)	14.419(18)	14.419(18)	14.419(18)	14.399(2)	C1A	0.0181(5)	0.0181(4)	0.0181(5)	0.0181(4)	0.0265(4)
c, Å	15.211(19)	15.212(19)	15.212(19)	15.212(19)	15.191(2)	C1B	0.0426(8)	0.0424(6)	0.0425(6)	0.0425(4)	0.0551(8)
N1 C1A	1.4760(7)	1.4758(6)	1.4758(5)	1.4759(4)	1.485(2)	C1'	0.0167(4)	0.0167(3)	0.0169(4)	0.0166(3)	0.0216(3)
C1A C1B	1.5248(10)	1.5251(7)	1.5250(6)	1.5248(4)	1.513(3)	O1'	0.0292(6)	0.0293(4)	0.0293(5)	0.0292(4)	0.0321(3)
C1A C1'	1.5127(6)	1.5125(5)	1.5125(5)	1.5125(4)	1.521(2)	N2	0.0180(3)	0.0181(2)	0.0181(3)	0.0180(2)	0.0267(3)
C1' O1'	1.2225(6)	1.2224(5)	1.2225(5)	1.2225(4)	1.229(2)	C2A	0.0213(4)	0.0213(3)	0.0213(3)	0.0213(2)	0.0257(4)
C1' N2	1.3394(6)	1.3394(5)	1.3392(4)	1.3393(4)	1.325(2)	C2'	0.0185(4)	0.0185(2)	0.0185(3)	0.0185(2)	0.0241(4)
N2 C2A	1.4432(6)	1.4432(6)	1.4432(5)	1.4432(3)	1.442(2)	O2'	0.0401(10)	0.0399(7)	0.0399(5)	0.0398(3)	0.0411(4)
C2A C2'	1.4944(6)	1.4946(4)	1.4945(5)	1.4945(4)	1.518(2)	N3	0.0147(3)	0.0147(2)	0.0147(2)	0.0147(2)	0.0239(3)
C2' N3	1.3316(6)	1.3315(5)	1.3316(5)	1.3315(4)	1.333(2)	C3A	0.0144(3)	0.0144(2)	0.0144(2)	0.0144(2)	0.0240(4)
C2' O2'	1.2170(5)	1.2172(5)	1.2171(5)	1.2170(5)	1.234(3)	C3B	0.0285(5)	0.0285(4)	0.0285(3)	0.0284(3)	0.0434(6)
N3 C3A	1.4415(5)	1.4416(5)	1.4415(4)	1.4414(4)	1.455(2)	C3'	0.0175(3)	0.0175(3)	0.0175(3)	0.0174(3)	0.0310(4)
C3A C3B	1.5260(7)	1.5260(5)	1.5262(5)	1.5262(4)	1.516(3)	O3'	0.0270(4)	0.0270(4)	0.0270(4)	0.0270(3)	0.0395(4)
C3A C3'	1.5478(6)	1.5478(5)	1.5477(5)	1.5477(4)	1.541(2)	O3	0.0366(7)	0.0366(6)	0.0365(5)	0.0365(5)	0.0641(6)
C3' O3	1.2410(6)	1.2412(5)	1.2411(4)	1.2411(4)	1.231(2)						
C3' O3'	1.2502(6)	1.2502(5)	1.2502(4)	1.2501(3)	1.260(2)						

Table S13. Effect of the size of simulation supercell on the simulation results.
AGA, length 2 ns.

geometry						Ueq					
parameter	360 at, cutoff 8	1920 at, cutoff 12	2880 at, cutoff 12	23040 at, cutoff 12	experiment	atom	360 at, cutoff 8	1920 at, cutoff 12	2880 at cutoff 12	23040 at cutoff 12	exp
a, Å	4.753(14)	4.754(6)	4.753(5)	4.753(2)	4.747(7)	N1	0.0207(6)	0.0272(8)	0.0272(5)	0.0291(3)	0.0315(4)
b, Å	14.417(42)	14.419(18)	14.418(14)	14.418(5)	14.399(2)	C1A	0.0150(3)	0.0181(5)	0.0185(3)	0.0204(2)	0.0265(4)
c, Å	15.210(44)	15.212(19)	15.212(15)	15.211(6)	15.191(2)	C1B	0.0361(6)	0.0425(6)	0.0435(4)	0.0458(5)	0.0551(8)
N1 C1A	1.4764(4)	1.4758(5)	1.4758(5)	1.4757(6)	1.485(2)	C1'	0.0132(3)	0.0169(4)	0.0170(3)	0.0190(2)	0.0216(3)
C1A C1B	1.5283(5)	1.5250(6)	1.5247(6)	1.5245(6)	1.513(3)	O1'	0.0265(4)	0.0293(5)	0.0296(4)	0.0317(3)	0.0321(3)
C1A C1'	1.5109(4)	1.5125(5)	1.5126(5)	1.5125(5)	1.521(2)	N2	0.0145(3)	0.0181(3)	0.0183(2)	0.0203(2)	0.0267(3)
C1' O1'	1.2210(5)	1.2225(5)	1.2224(5)	1.2224(5)	1.229(2)	C2A	0.0187(5)	0.0213(3)	0.0215(2)	0.0235(3)	0.0257(4)
C1' N2	1.3398(4)	1.3392(4)	1.3394(5)	1.3394(5)	1.325(2)	C2'	0.0134(4)	0.0185(3)	0.0187(2)	0.0205(2)	0.0241(4)
N2 C2A	1.4451(5)	1.4432(5)	1.4432(4)	1.4432(5)	1.442(2)	O2'	0.0282(5)	0.0399(5)	0.0402(6)	0.0423(6)	0.0411(4)
C2A C2'	1.4965(4)	1.4945(5)	1.4945(5)	1.4945(5)	1.518(2)	N3	0.0119(3)	0.0147(2)	0.0148(2)	0.0166(2)	0.0239(3)
C2' N3	1.3393(3)	1.3316(5)	1.3315(4)	1.3313(5)	1.333(2)	C3A	0.0114(5)	0.0144(2)	0.0146(2)	0.0164(2)	0.0240(4)
C2' O2'	1.2194(5)	1.2171(5)	1.2170(5)	1.2169(5)	1.234(3)	C3B	0.0245(6)	0.0285(3)	0.0285(3)	0.0307(3)	0.0434(6)
N3 C3A	1.4484(3)	1.4415(4)	1.4416(4)	1.4414(5)	1.455(2)	C3'	0.0127(6)	0.0175(3)	0.0176(2)	0.0194(2)	0.0310(4)
C3A C3B	1.5267(4)	1.5262(5)	1.5261(6)	1.5261(5)	1.516(3)	O3'	0.0198(8)	0.0270(4)	0.0270(3)	0.0292(3)	0.0395(4)
C3A C3'	1.5423(5)	1.5477(5)	1.5477(5)	1.5476(5)	1.541(2)	O3	0.0310(8)	0.0365(5)	0.0367(4)	0.0389(4)	0.0641(6)
C3' O3	1.2399(7)	1.2411(4)	1.2410(5)	1.2410(5)	1.231(2)						
C3' O3'	1.2485(5)	1.2502(4)	1.2502(4)	1.2501(5)	1.260(2)						

Table S14. Ueq for AGA 3192 mol (95760 atoms)
length 0.5 ns, cutoff 12

atom	0-100000	100000-200000	200000-300000	300000-400000	400000-500000	ave	exp
N1	0.0295(11)	0.0297(11)	0.0296(11)	0.0297(11)	0.0296(11)	0.0296(11)	0.0315(4)
C1A	0.0210(8)	0.0211(8)	0.0210(8)	0.0211(7)	0.0210(8)	0.0210(8)	0.0265(4)
C1B	0.0462(19)	0.0464(19)	0.0464(19)	0.0464(18)	0.0464(19)	0.0464(19)	0.0551(8)
C1'	0.0195(8)	0.0196(7)	0.0196(7)	0.0197(8)	0.0196(8)	0.0196(8)	0.0216(3)
O1'	0.0321(12)	0.0323(12)	0.0322(12)	0.0323(12)	0.0322(12)	0.0322(12)	0.0321(3)
N2	0.0208(8)	0.0209(7)	0.0209(7)	0.0210(8)	0.0209(7)	0.0209(7)	0.0267(3)
C2A	0.0240(10)	0.0241(10)	0.0240(9)	0.0241(10)	0.0240(9)	0.0240(10)	0.0257(4)
C2'	0.0210(9)	0.0211(9)	0.0211(9)	0.0211(9)	0.0211(9)	0.0211(9)	0.0241(4)
O2'	0.0426(23)	0.0428(23)	0.0428(23)	0.0428(23)	0.0428(23)	0.0428(23)	0.0411(4)
N3	0.0171(6)	0.0172(6)	0.0172(6)	0.0172(6)	0.0172(6)	0.0172(6)	0.0239(3)
C3A	0.0169(6)	0.0170(6)	0.0170(6)	0.0171(6)	0.0170(6)	0.0170(6)	0.0240(4)
C3B	0.0311(11)	0.0313(11)	0.0313(11)	0.0313(11)	0.0312(11)	0.0312(11)	0.0434(6)
C3'	0.0199(8)	0.0200(8)	0.0200(8)	0.0201(8)	0.0197(8)	0.0199(8)	0.0310(4)
O3'	0.0294(11)	0.0295(11)	0.0295(11)	0.0295(11)	0.0294(11)	0.0295(11)	0.0395(4)
O3	0.0390(16)	0.0392(16)	0.0392(15)	0.0392(16)	0.0391(16)	0.0391(16)	0.0641(6)

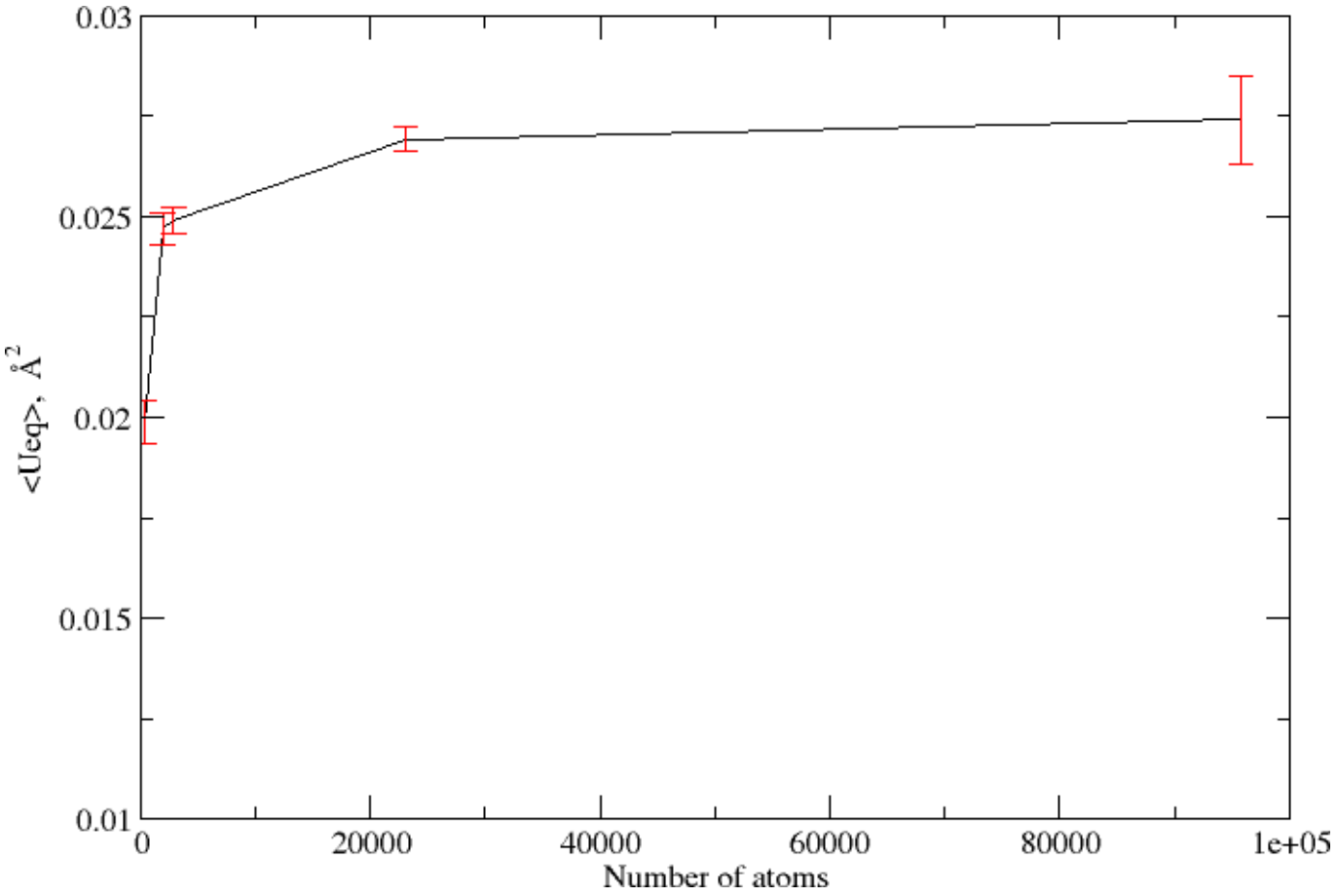

Figure S2. Effect of the size of the size of simulation supercell on the simulation results. It can be seen that the Ueq are converging.

Table S15. Effect of cutoff for non-bonded interactions on the simulation results.

AGA 768 mol (23040 atoms), length 2 ns, unless otherwise specified

geometry						Ueq					
parameter	cutoff 12	cutoff 16	cutoff 20	cutoff 24 (1 ns)	experiment	atom	cutoff 12	cutoff 16	cutoff 20	cutoff 24 (1 ns)	exp
a, Å	4.753(2)	4.752(2)	4.751(2)	4.751(2)	4.747(7)	N1	0.0291(3)	0.0290(3)	0.0290(3)	0.0290(3)	0.0315(4)
b, Å	14.418(5)	14.414(5)	14.412(5)	14.412(5)	14.399(2)	C1A	0.0204(2)	0.0204(2)	0.0204(2)	0.0204(2)	0.0265(4)
c, Å	15.211(6)	15.207(5)	15.205(6)	15.204(5)	15.191(2)	C1B	0.0458(5)	0.0457(5)	0.0457(5)	0.0457(5)	0.0551(8)
N1 C1A	1.4757(6)	1.4757(6)	1.4757(6)	1.4757(6)	1.485(2)	C1'	0.0190(2)	0.0189(2)	0.0189(2)	0.0189(2)	0.0216(3)
C1A C1B	1.5245(6)	1.5245(6)	1.5245(6)	1.5245(6)	1.513(3)	O1'	0.0317(3)	0.0315(4)	0.0316(3)	0.0316(3)	0.0321(3)
C1A C1'	1.5125(5)	1.5125(5)	1.5125(5)	1.5125(5)	1.521(2)	N2	0.0203(2)	0.0202(2)	0.0202(2)	0.0202(2)	0.0267(3)
C1' O1'	1.2224(5)	1.2224(5)	1.2224(5)	1.2224(5)	1.229(2)	C2A	0.0235(3)	0.0234(3)	0.0234(2)	0.0234(2)	0.0257(4)
C1' N2	1.3394(5)	1.3394(5)	1.3394(5)	1.3394(5)	1.325(2)	C2'	0.0205(2)	0.0205(2)	0.0205(2)	0.0205(2)	0.0241(4)
N2 C2A	1.4432(5)	1.4432(5)	1.4432(5)	1.4432(5)	1.442(2)	O2'	0.0423(6)	0.0422(6)	0.0422(6)	0.0422(6)	0.0411(4)
C2A C2'	1.4945(5)	1.4945(5)	1.4945(5)	1.4945(5)	1.518(2)	N3	0.0166(2)	0.0165(2)	0.0165(2)	0.0165(2)	0.0239(3)
C2' N3	1.3313(5)	1.3313(5)	1.3313(5)	1.3313(5)	1.333(2)	C3A	0.0164(2)	0.0163(2)	0.0163(2)	0.0163(2)	0.0240(4)
C2' O2'	1.2169(5)	1.2169(5)	1.2169(5)	1.2169(5)	1.234(3)	C3B	0.0307(3)	0.0305(3)	0.0305(3)	0.0305(3)	0.0434(6)
N3 C3A	1.4414(5)	1.4414(5)	1.4414(5)	1.4414(5)	1.455(2)	C3'	0.0194(2)	0.0193(2)	0.0193(2)	0.0193(2)	0.0310(4)
C3A C3B	1.5261(5)	1.5261(5)	1.5261(5)	1.5261(5)	1.516(3)	O3'	0.0292(3)	0.0288(60)	0.0288(99)	0.0288(3)	0.0395(4)
C3A C3'	1.5476(5)	1.5476(5)	1.5476(5)	1.5476(5)	1.541(2)	O3	0.0389(4)	0.0385(59)	0.0385(99)	0.0385(4)	0.0641(6)
C3' O3	1.2410(5)	1.2410(5)	1.2410(5)	1.2410(5)	1.231(2)						
C3' O3'	1.2501(5)	1.2501(5)	1.2501(5)	1.2501(5)	1.260(2)						